Non-perturbative calculation of the two-loop Lamb shift in Li-like ions

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A calculation valid to all orders in the nuclear-strength parameter is presented for the two-loop Lamb shift, notably for the two-loop self-energy correction, to the $2p$-$2s$ transition energies in heavy Li-like ions. The calculation removes the largest theoretical uncertainty for these transitions and yields the first experimental identification of two-loop QED effects in the region of the strong binding field.

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The Coulomb field of heavy nuclei provides a unique opportunity for testing the strong-field regime of bound-state quantum electrodynamics (QED). The most obvious candidate for such a test is an H-like ion, whose theoretical description is the simplest one. Measurements of the $1s$ Lamb shift in H-like uranium, the heaviest naturally occurring element, have recently achieved an accuracy of 4.6 eV [1]. This corresponds to a fractional accuracy of 1.7% with respect to the total $1s$ QED contribution. Such measurements yield a test of bound-state QED at the one-loop level (i.e., to first order in the fine structure constant α), but they are yet insensitive to the *two-loop* QED corrections, which are of primary theoretical interest at present.

By contrast, measurements of the $2p$-$2s$ transition energies in heavy Li-like ions [2, 3, 4, 5] have lately reached a fractional accuracy of 0.03% with respect to the total QED contribution. This corresponds to a 10% sensitivity of the experimental results to the two-loop QED contribution. These measurements provide an excellent possibility for identification of the two-loop Lamb shift and for testing the bound-state QED up to second order in α in the strong-field regime.

The theoretical description of Li-like ions is complicated by the presence of the electron-electron interaction. For heavy ions, this interaction can be successfully accounted for within the perturbative expansion in a small parameter $1/Z$ (Z is the nuclear charge number). By calculating a few terms of this expansion, one can rigorously describe the electron correlation and the screening of one-loop QED corrections with the accuracy sufficient for identification of the two-loop Lamb shift. Such a project has recently been accomplished in [6, 7]. Based on these calculations, an "experimental" value of -0.23 eV was inferred in [5] for the $2s$ two-loop Lamb shift in Li-like uranium. A similar determination of the two-loop Lamb shift was earlier presented in [7] (based on the measurement [3]) for the $2p_{3/2}$-$2s$ transition energy in bismuth.

The subject of our present interest is the set of two-loop one-electron QED corrections (also referred to as the two-loop Lamb shift), graphically represented in Fig. 1. These corrections have lately been extensively investigated within the perturbative expansion in the nuclear-strength parameter $Z\alpha$ [8, 9, 10, 11, 12]. Such studies, however, do not provide reliable information about the magnitude of the two-loop Lamb shift in heavy ions like uranium, where the parameter $Z\alpha$ approaches unity. Our present investigation is addressed primarily to high-Z ions and will be performed non-perturbatively, i.e., without an expansion in $Z\alpha$. The only exception will be made for the diagrams in Fig. 1(h)-(k), for which we will expand the fermion loops in terms of the binding potential. We will keep the leading term of the expansion and refer to this as the free-loop approximation. In the one-loop case, such approximation corresponds to the Uehling potential and yields the dominant contribution even for high-Z ions like uranium.

Necessity for a non-perturbative calculation of the two-loop Lamb shift became clear already in the beginning of the 1990s, after the famous measurement [2] of the $2p_{1/2}$-$2s$ transition energy in U^{89+} with an accuracy of 0.1 eV. Quite soon, calculations of all diagrams in Fig. 1(d)-(k) were accomplished [13] [although the graphs (i) and (k) were calculated in the free-loop approximation only]. Three remaining diagrams (a)-(c), referred to as the two-loop self-energy correction, turned out to be much more difficult to evaluate. The calculation for the $1s$ state extended over a decade [14, 15, 16], with the first complete evaluation presented in [17] and later extended in [18].

In this Letter, we present our calculation of the two-loop self-energy correction for the $2s$, $2p_{1/2}$, and $2p_{3/2}$ states of several high-Z ions. We also evaluate the remaining diagrams

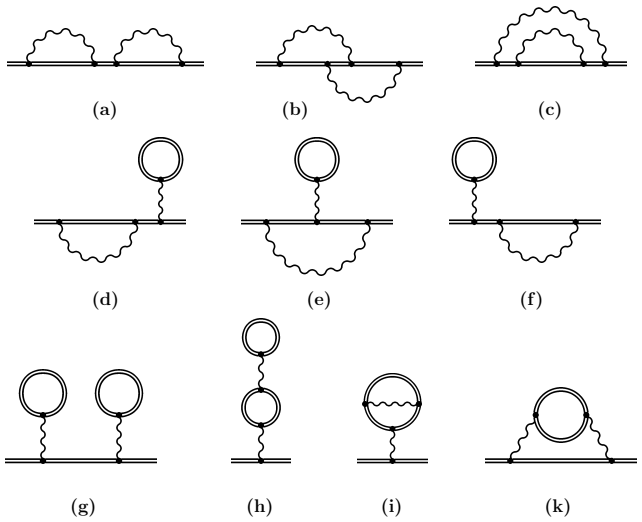

FIG. 1: Two-loop one-electron QED corrections. Gauge-invariant subsets are referred to as SESE (a-c), SEVP (d-f), VPVP (g-i), S(VP)E (k).

TABLE I: The two-loop self-energy correction, in terms of $F(Z\alpha)$.

Z	$1s$	$2s$	$2p_{1/2}$	$2p_{3/2}$
60	$-1.666\,(19)$	$-1.976\,(70)$	$0.222\,(72)$	$0.02\,(14)$
70	$-1.923\,(18)$	$-2.453\,(60)$	$0.192\,(60)$	$-0.082\,(93)$
83	$-2.360\,(15)$	$-3.296\,(38)$	$0.133\,(38)$	$-0.175\,(66)$
92	$-2.806\,(12)$	$-4.218\,(34)$	$0.012\,(32)$	$-0.241\,(48)$
100	$-3.392\,(14)$	$-5.455\,(68)$	$-0.214\,(32)$	$-0.282\,(52)$

in Fig. 1 and obtain results for the total two-loop Lamb shift, this being previously the largest uncalculated correction for the $2p$-$2s$ transition energies in heavy Li-like ions. Our calculation significantly refines theoretical predictions for these transition energies and provides a test of bound-state QED theory in the strong-field regime up to second order in α.

Another important aspect of our calculations is associated with their implications for the hydrogen Lamb shift. In the previous evaluation of the $1s$ two-loop self-energy correction [18], we demonstrated that an extrapolation of our results to $Z = 1$ yields a value that disagrees with the analytical result to order $\alpha^2(Z\alpha)^6$ [11]. In view of this disagreement, it will be of interest to compare our non-perturbative values with the analytical result to order $\alpha^2(Z\alpha)^6$ for the normalized difference of the $2s$ and $1s$ energy shifts, $\Delta_s = 8\,\delta E_{2s} - \delta E_{1s}$. Such a comparison can provide us with new information about the discrepancy for the $1s$ state, since, within the perturbative approach, the difference Δ_s is understood much better than the energy shift of a single ns state [19].

The calculational scheme for the evaluation of the two-loop self-energy correction was developed for the ground state in our previous studies [17, 18]. With this work, we extend it to the excited states. The general procedure for isolation and cancelation of divergences is similar to that for the $1s$ state, but the actual calculational scheme requires substantial modifications due to a more complicated pole and angular-momentum structure of expressions involved. Details of our calculation will be published elsewhere; in this Letter we concentrate on presentation and analysis of the results obtained.

The two-loop self-energy correction to the energy is conveniently represented in terms of the function F defined by

$$\delta E = mc^2 \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\,\alpha)^4}{n^3}\, F(Z\,\alpha)\,, \qquad (1)$$

where n is the principal quantum number. The numerical results obtained for the $n = 1$ and 2 states are listed in Table I. The calculation was performed for the point model of the nuclear-charge distribution.

As an intermediate step in our calculation, we had to consider the irreducible part of the diagram in Fig. 1(a), also denoted as the loop-after-loop correction, previously calculated in [14]. We report a good agreement with the previous results for the $1s$ state but find a discrepancy for $2s$ and $2p_{1/2}$ states. For $Z = 92$, we obtain -0.090 eV and -0.030 eV for the $2s$ and the $2p_{1/2}$ state, respectively, which should be compared with the values of -0.069 eV and 0.014 eV from [14], respectively. The apparent reason for this disagreement is a sign error in the contribution due to the imaginary part of the self-energy operator.

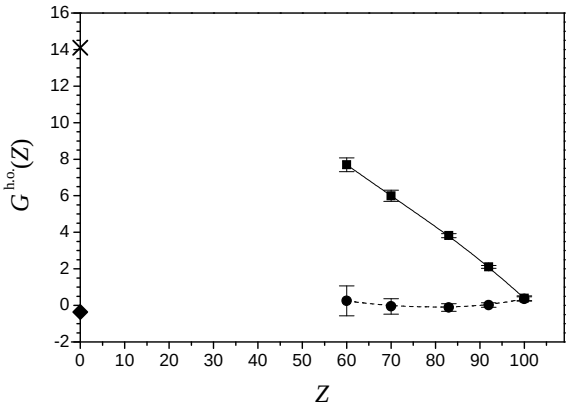

FIG. 2: Non-perturbative results for the higher-order remainder $G^{\rm h.o.}(Z)$ for the differences Δ_s (squares) and Δ_p (dots) and their limiting values at $Z = 0$ denoted by the cross for Δ_s and by the diamond for Δ_p.

The consistency of our numerical values can be tested by comparing them with analytical results obtained within the perturbative approach. The $Z\alpha$ expansion of the function F reads

$$F(Z\alpha) = B_{40} + (Z\alpha)\,B_{50} + (Z\alpha)^2\left[L^3\,B_{63} + L^2\,B_{62} + L\,B_{61} + G^{\rm h.o.}(Z\alpha)\right], \qquad (2)$$

where $L = \ln[(Z\alpha)^{-2}]$ and $G^{\rm h.o.}$ is the remainder, $G^{\rm h.o.}(Z\alpha) = B_{60} + Z\alpha\,(\cdots)$. The coefficients B_{40}-B_{61} are presently known for all states of our interest [8, 9, 12]. The coefficient B_{60} was calculated for the specific differences of energy shifts $\Delta_s = 8\,\delta E_{2s} - \delta E_{1s}$ and $\Delta_p = \delta E_{2p_{3/2}} - \delta E_{2p_{1/2}}$ [10, 12]. A calculation of the dominant part of $B_{60}(1s)$ and $B_{60}(2s)$ was reported in [11], together with an estimate of unevaluated contributions to this order.

We would like now to isolate the contribution of the higher-order remainder $G^{\rm h.o.}$ from our numerical results. Obviously, such isolation leads to a significant loss of precision, which grows fast when Z decreases. Moreover, the data presented in Table I for the function F are already a result of a significant (and Z-dependent) cancelation, since individual contributions to the energy do not exhibit the physical Z^4 dependence but scale typically as Z or Z^2. This indicates that an analysis of the Z behavior of the higher-order remainder $G^{\rm h.o.}$ provides a stringent test of the consistency of the numerical results.

In Fig. 2, we present our results for the higher-order remainder $G^{\rm h.o.}(Z)$ for the differences Δ_s and Δ_p, together with their limiting values $G^{\rm h.o.}(0) = B_{60}$, which are $14.1(4)$ for Δ_s and -0.3611 for Δ_p [10, 12]. The comparison presented in the figure indicates that our non-perturbative results are in good qualitative agreement with the perturbative expansion coefficients known for the differences Δ_s and Δ_p. A quantitative comparison is presently impossible due to a lack of numerical data in the low-Z region. To perform a non-perturbative calculation for excited states of low-Z ions is a

TABLE II: Individual two-loop contributions to transition energies in Li-like bismuth and uranium, in eV.

Subset	Fig.	$2p_{3/2}$-$2s$, $Z=83$	$2p_{1/2}$-$2s$, $Z=92$
SESE	(a)-(c)	0.145 (4)	0.296 (3)
SEVP	(d)-(f)	−0.095	−0.187
VPVP	(g)	0.016	0.035
VPVP	(h),(i)	0.067 (25)	0.101 (46)
S(VP)E	(k)	−0.012 (24)	−0.022 (45)
Total		0.120 (35)	0.223 (64)

TABLE III: Various contributions to transition energies in Li-like bismuth and uranium, in eV.

	$2p_{3/2}$-$2s$, $Z=83$	$2p_{1/2}$-$2s$, $Z=92$
Dirac value	2792.21 (3)	−33.27 (9)
One-photon exchange	23.82	368.83
Two-photon exchange	−1.61	−13.37
Three-photon exchange	−0.02 (2)	0.15 (7)
One-loop QED	−27.48	−42.93
Screened QED	1.15 (4)	1.16 (3)
Two-loop QED	0.12 (4)	0.22 (6)
Recoil	−0.07	−0.07
Nuclear polarization		0.04 (2)
Total theory	2788.12 (7)	280.76 (14)
Experiment	2788.14 (4) [3]	280.645 (15) [5]

difficult problem, whose solution apparently requires development of new calculational technique. For the $1s$ state, however, such a calculation is less problematic and we were able to carry out a direct evaluation for Z as low as 10 in our previous investigation [18]. Extrapolating our $1s$ results to $Z=1$ in that work, we found a disagreement with the analytical value for the coefficient $B_{60}(1s)$ [11]. Our present calculation for the difference Δ_s and the agreement observed with the analytical expansion coefficients in this case can be considered as an evidence in favor of reliability of our previous results for the $1s$ state.

In Table II, we present the results of our calculations of all two-loop corrections depicted in Fig. 1 for the $2p_{3/2}$-$2s$ transition in Bi^{80+} and the $2p_{1/2}$-$2s$ transition in U^{89+}, for which most accurate experimental data are available. The contribution of the SESE subset is taken from Table I. The diagrams in Fig. 1(d)-(g) were calculated rigorously to all orders in $Z\alpha$, whereas the diagrams in Fig. 1(h)-(k) were evaluated within the free-loop approximation, i.e., keeping the first nonvanishing contribution in the expansion of the fermion loops in terms of the binding potential. The error bars specified for these corrections are estimations of uncertainty due to the approximation employed. They were obtained by multiplying the contribution of Fig. 1(h,i) by a factor of $(Z\alpha)^2$ and that of Fig. 1(k), by a factor of $3\,(Z\alpha)$. The factor of $3\,(Z\alpha)$ in the latter estimation arises as a ratio of the leading-order contribution beyond the free-loop approximation for the diagram (k), $-0.386\,(\alpha/\pi)^2(Z\alpha)^5$ [20], and the leading-order contribution within this approximation, $0.142\,(\alpha/\pi)^2(Z\alpha)^4$ [21]. The finite nuclear size effect was taken into account in our evaluation of the diagrams in Fig. 1(d)-(i), whereas the other diagrams were calculated for the point nuclear model. In the case of uranium, our results for the diagrams with closed fermion loops are in good agreement with those reported previously [22].

We now turn to the experimental consequences of our calculations. In Table III, we collect all available theoretical contributions to the the $2p_{3/2}$-$2s$ transition energy in Bi^{80+} and to the $2p_{1/2}$-$2s$ transition energy in U^{89+}. The entry labeled "Dirac value" represents the transition energies as obtained from the Dirac equation with the Fermi-like nuclear potential and the nuclear-charge root-mean-square (rms) radius fixed as $<r^2>^{1/2}= 5.851(7)$ Fm for uranium and $5.521(3)$ Fm for bismuth [23]. The dependence of the Dirac value on the nuclear model was conservatively estimated by comparing the results obtained within the Fermi and the homogeneously-charged-sphere models [24]. We have checked that a wide class of more general models for the nuclear-charge distribution yields results well within the error bars obtained in this way.

The next 3 lines contain the corrections due to the one-, two-, and three-photon exchange, respectively. QED values for the two-photon exchange correction were taken from our previous evaluations [6, 25]. The results for the three-photon exchange correction were obtained in this work within many-body perturbation theory (MBPT), with retaining the Breit interaction to the first order only. For uranium, we report good agreement with the previous evaluations of this effect [26]. The error ascribed to the three-photon exchange correction is due to incompleteness of the MBPT treatment. It was estimated by calculating the third-order MBPT contribution with two and more Breit interactions for each state involved in the transition, adding these contributions quadratically, and multiplying the result by a conservative factor of 2.

The entry labeled "One-loop QED" represents the sum of the first-order self-energy and vacuum-polarization corrections calculated on hydrogenic wave functions [22]. The next line ("Screened QED") contains the results for the screened self-energy and vacuum-polarization corrections [27]. The uncertainty ascribed to this entry is the estimation of higher-order screening effects; it was obtained by multiplying the correction by the ratio of the entries "Screened QED" and "One-loop QED". The entry "Two-loop QED" contains the results for the two-loop Lamb shift obtained in the present investigation. The next two lines contain the values for the relativistic recoil correction [28] and the nuclear polarization correction [29].

Table III shows that now, after our calculation of the two-loop Lamb shift, the total theoretical uncertainty is significantly influenced by the error of the finite-nuclear-size effect. It should be noted that a certain concern exists in the community about the accuracy of the theoretical description of this correction. In particular, it was pointed out [30] that little is known about systematical effects in experimental determination of nuclear rms radii. In the absence of detailed investigations of such effects, we consider the errors of rms radii obtained in [23] by averaging all experimental results available (including both muonic-ions and electron-scattering data) to

be presently the most reliable estimates and employ these values in our calculations.

The comparison presented in Table III demonstrates that our total results agree well within the error bars specified with the experimental data for bismuth and uranium. The theoretical accuracy is significantly better in the former case, which is the consequence of the fact that the finite nuclear size effect is smaller and the nuclear radius is known better. Our result for the $2p_{3/2}$-$2s$ transition in bismuth can also be compared with the value of 2787.96 eV obtained by Sapirstein and Cheng [7]. The difference of 0.16 eV between the results is mainly due to the two-loop Lamb shift contribution (0.12 eV) which is not accounted for in [7].

We conclude that inclusion of the two-loop Lamb shift is necessary for adequate interpretation of the experimental result in the case of bismuth, whereas for uranium the two-loop Lamb shift is significantly screened by the uncertainty due to the nuclear charge distribution. Comparison of the theoretical and experimental results for bismuth yields the first identification of the two-loop QED effects in the region of strong binding field, which is the first step toward the test of the strong-field regime of bound-state QED at the two-loop level.

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[1] A. Gumberidze *et al.* Phys. Rev. Lett. **94**, 223001 (2005).
[2] J. Schweppe *et al.* Phys. Rev. Lett. **66**, 1434 (1991).
[3] P. Beiersdorfer *et al.* Phys. Rev. Lett. **80**, 3022 (1998).
[4] C. Brandau *et al.* Phys. Rev. Lett. **91**, 073202 (2003).
[5] P. Beiersdorfer *et al.* Phys. Rev. Lett. **95**, 233003 (2005).
[6] V. A. Yerokhin *et al.* Phys. Rev. Lett. **85**, 4699 (2000); Phys. Rev. A **64**, 032109 (2001).
[7] J. Sapirstein and K. T. Cheng, Phys. Rev. A **64**, 022502 (2001).
[8] K. Pachucki, Phys. Rev. Lett. **72**, 3154 (1994); M. Eides and V. Shelyuto, Phys. Rev. A **52**, 954 (1995); S. Karshenboim, J. Phys. B **29**, L29 (1996).
[9] K. Pachucki, Phys. Rev. A **63**, 042503 (2001).
[10] U. D. Jentschura and K. Pachucki, J. Phys. A **35**, 1927 (2002).
[11] K. Pachucki and U. D. Jentschura, Phys. Rev. Lett. **91**, 113005 (2003).
[12] A. Czarnecki, U. D. Jentschura, and K. Pachucki, Phys. Rev. Lett. **95**, 180404 (2005); U. D. Jentschura, A. Czarnecki, and K. Pachucki, Phys. Rev. A **72**, 062102 (2005).
[13] T. Beier and G. Soff, Z. Phys. D **8**, 129 (1988); H. Persson *et al.* Phys. Rev. A **54**, 2805 (1996); S. Mallampalli and J. Sapirstein, Phys. Rev. A **54**, 2714 (1996); G. Plunien *et al.* Eur. Phys. J. D **1**, 177 (1998).
[14] A. Mitrushenkov *et al.* Phys. Lett. **A200**, 51 (1995).
[15] S. Mallampalli and J. Sapirstein, Phys. Rev. A **57**, 1548 (1998).
[16] V. A. Yerokhin and V. M. Shabaev, Phys. Rev. A **64**, 062507 (2001).
[17] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Phys. Rev. Lett. **91**, 073001 (2003); Eur. Phys. J. D **25**, 203 (2003).
[18] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Phys. Rev. A **71**, 040101(R) (2005); JETP **101**, 280 (2005).
[19] S. G. Karshenboim, JETP **78**, 230 (1994).
[20] K. Pachucki, Phys. Rev. A **48**, 2609 (1993).
[21] B. E. Lautrup *et al.*, Phys. Lett. **B31**, 577 (1970); R. Barbieri *et al.*, Nuovo Cimento Lett. **3**, 588 (1970).
[22] P. J. Mohr, G. Plunien, and G. Soff, Phys. Rep. **293**, 227 (1998).
[23] I. Angeli, At. Data Nucl. Data Tables **87**, 185 (2004).
[24] T. Franosch and G. Soff, Z. Phys. D **18**, 219 (1991).
[25] A. N. Artemyev *et al.* Phys. Rev. A **67**, 062506 (2003).
[26] O. M. Zherebtsov, V. M. Shabaev, and V. A. Yerokhin, Phys. Lett. A **277**, 227 (2000); O. Yu. Andreev *et al.* Phys. Rev. A **64**, 042513 (2001).
[27] A. N. Artemyev *et al.* Phys. Rev. A **60**, 45 (1999); V. A. Yerokhin *et al.* Phys. Rev. A **60**, 3522 (1999); V. A. Yerokhin *et al.* Optics and Spectroscopy **99**, 12 (2005).
[28] A. N. Artemyev, V. M. Shabaev, and V. A. Yerokhin, Phys. Rev. A **52**, 1884 (1995); J. Phys. B **28**, 5201 (1995).
[29] G. Plunien and G. Soff, Phys. Rev. A **51**, 1119 (1995); *ibid* **53**, 4614 (1996); A. V. Nefiodov *et al.* Phys. Lett. A **222**, 227 (1996).
[30] S. G. Karshenboim, Phys. Rep. **422**, 1 (2005).